<States and Structures> Atomic and Molecular Physics

States and Structures
- Atomic and Molecular Physics -

http://elec.kuicr.kyoto-u.ac.jp

Prof
HATA, Yasuo
(D Sc)

Assoc Prof
ITO, Yoshiaki
(D Sc)

Instr
NAKAMATSU, Hirohide
(D Sc)

Instr
FUJII, Tomomi
(D Sc)

A Res
TOCHIO, Tatsunori
(D Sc)

Students

OoHASHI, Hirofumi (D3)
HAYASHIDA, Minoru (D3)
SAKAKURA, Shusuke (M1)
MIZOTA, Hirohisa (M1)

Visitors

Prof FRICKE, Burkhard — University of Kassel, Germany, 10-11 March 2003
Dr SHARMA, Sangeeta — Institute of Theoretical Physics, University of Graz, Austria, 8-18 September 2003

Scope of Research

The research activities in this laboratory are performed for X-ray structural analyses of biological macromolecules and inorganic materials as follows. The main subjects of the biomacromolecular crystallography are crystallographic studies on the reaction mechanism of enzymes, the relationship between the multiform conformation and the functional variety of proteins, and the mechanism of thermostabilization of proteins. In the structural analyses of inorganic materials, the electronic states of atoms and molecules are investigated in detail using conventional X-ray and SR in order to obtain fundamental information on the property and structure of materials. The theoretical analysis of the electronic states and the development of new radiation detectors are also performed.

Research Activities (Year 2003)

Presentations

Crystallographic analyses of enzyme functions in the field of agricultural chemistry; Hata Y, Annual Meeting, Jpn. Soc. Biosci. Biotech. AgroChem., 3 April.

Similarities between protein-protein and protein-carbohydrate interactions of pokeweed lectins; Hayashida M, Fujii T, Ishiguro M (Kyushu), Hata Y, Annual Meeting, Prot. Sci. Soc. Jpn., 25 June.

Crystal structure of thermostable aspartase and structure-based exploration of functional sites in the aspartase family; Hata Y, Fujii T, Sakai H, Kawata Y (Tottori), Broome2003 Int. Crystallography Meetings AsCA'03/Crystal-23, 12 August.

$K\alpha$ x-ray emission spectra of Cr compounds; Tochio T, Ito Y, Sherman E Y, Ambrosch-Draxl C, Vlaicu A M, Fukushima S, Shoji T, Nineth Wien-Workshop, Vienna, Austria, April 23-26, 2003.

Grants

Hata Y, Protein-engineering studies on the unique conformations and the expression mechanism of function of pokeweed lectines, Grant-in-Aid for Scientific Research on Priority Areas (C) (2), 1 April 2002 - 31 March 2004.

Hata Y, Structural analyses of gene-products involved in protein structure formation, Protein 3000 Project, 1 April 2002 - 31 March 2007.

Fujii T, Elucidation of mechanism of structural change in functional sites of aspartase, Grant-in-Aid for Young Scientists (B), 1 April 2003 - 31 March 2005.

X-ray crystal structure analysis of pokeweed lectin PL-C

Pokeweed lectin (PL) is a mitogenic lectin, which is specific for *N*-acetylglucosamine-containing saccharides and exceptionally activates both T and B cells. Five lectins, designated PL-A, PL-B, PL-C, PL-D1, and PL-D2, have been isolated from the roots of pokeweed. PL-C is a mitogen but exhibits no heamagglutinating activity. The polypeptide chain of PL-C consists of three chitin-binding domains, each of which has four S-S bridges and the putative saccharide-binding site.

The crystal structure of PL-C has been solved by the isomorphous replacement method and refined up to 1.8 Å resolution with the *R*-factor of 17.6%. Two subunits in the asymmetric unit of the PL-C crystal are related to each other by the non-crystallographic 2-fold axis and form a dimer in a head-to-tail fashion with three pairs of putative carbohydrate-binding sites facing each other (Figure 1). All the sites in the subunit are located in the dimer interface. The dimerization of PL-C is performed through the hydrophobic interactions between the putative carbohydrate-binding sites of opposite domains in the dimer. The PL-C dimer has no room for accommodating the carbohydrate. Therefore, the loss of carbohydrate-binding ability due to self-association probably the reason that PL-C exhibits no agglutinating activity.

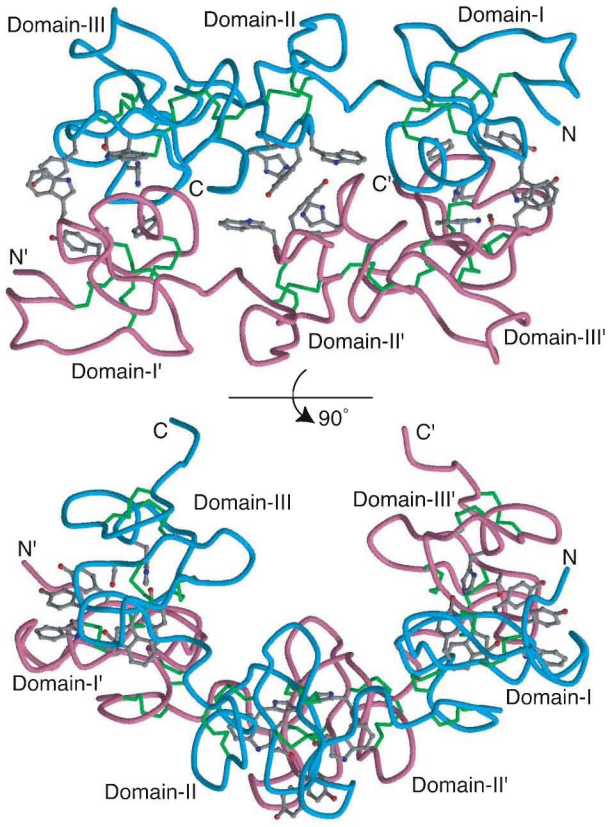

Figure 1. The PL-C dimer structure.

Photon cooking

The third generation synchrotron radiation such as SPring-8 is very intense and tunable x-ray source, and offers detailed photoexcitation measurements around the threshold regions. Especially, X-ray emission spectroscopy is a suitable tool to study the satellites due to the electron correlation.

Pt $L\beta_{15}$ ($L_{III} \rightarrow N_{IV}$) emission line has not been yet confirmed due to the overlap of Pt $L\beta_3$ ($L_I \rightarrow M_{III}$) diagram line. However, the energy value of Pt $L\beta_{15}$ emission can be obtained using a high resolution X-ray spectrometer with tunable photon energies around L_I threshold.

The incident photon energy was scanned in the energy range around the Pt L_I edge. Two excitation energies were used below and above the L_I edge (13880.7 eV). Pt $L\beta_{15}$ emission line overlaps $L\beta_3$ line above the edge, only Pt $L\beta_{15}$ diagram line could finally be obtained below the edge as seen in figure 2. It took more than a half century to get this value.

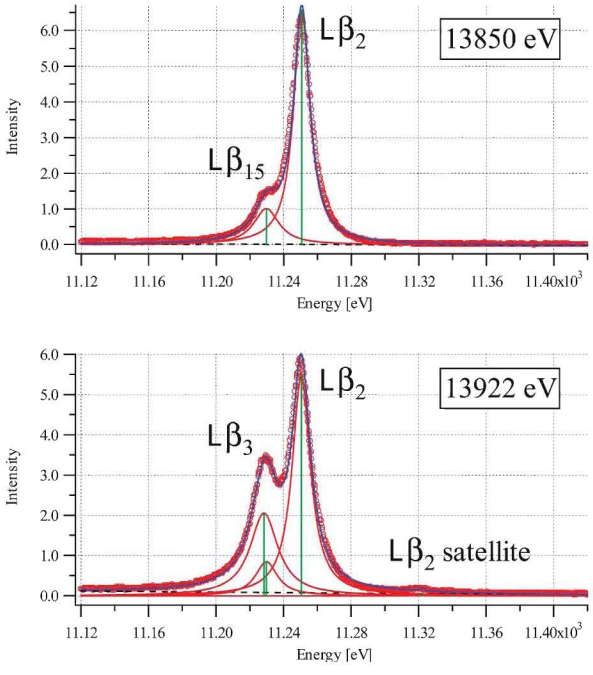

Figure 2. Pt $L\beta_{2,3,15}$ obtained below and above L_I edge